

Exactly solvable reaction diffusion models on a Cayley tree

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Abstract

The most general reaction-diffusion model on a Cayley tree with nearest-neighbor interactions is introduced, which can be solved exactly through the empty-interval method. The stationary solutions of such models, as well as their dynamics, are discussed. Concerning the dynamics, the spectrum of the evolution Hamiltonian is found and shown to be discrete, hence there is a finite relaxation time in the evolution of the system towards its stationary state.

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1 Introduction

Reaction-diffusion systems have been studied using various methods, including analytical techniques, approximation methods, and simulation. Approximation methods are generally different in different dimensions, as for example the mean field techniques, working good for high dimensions, generally do not give correct results for low-dimensional systems. A large fraction of analytical studies belong to low-dimensional (specially one-dimensional) systems, as solving low-dimensional systems should in principle be easier. [1–11].

The Cayley tree is a tree (a lattice having no loops) where every site is connected to ξ nearest neighbor sites. This no-loops property may allow exact solvability for some models, for general coordination number ξ . Reaction diffusion models on the Cayley tree have been studied in, for example [12–17]. In [12,13,16] diffusion-limited aggregations, and in [14] two-particle annihilation reactions for immobile reactants have been studied. There are also some exact results for deposition processes on the Bethe lattice [17].

The empty interval method (EIM) has been used to analyze the one dimensional dynamics of diffusion-limited coalescence [18–21]. Using this method, the probability that n consecutive sites are empty has been calculated. This method has been used to study a reaction-diffusion process with three-site interactions [22]. EIM has been also generalized to study the kinetics of the q -state one-dimensional Potts model in the zero-temperature limit [23]. In [18–21], one-dimensional diffusion-limited processes have been studied using EIM. There, some of the reaction rates have been taken infinite, and the models have been worked out on continuum. For the cases of finite reaction-rates, some approximate solutions have been obtained.

In [24, 25], all the one dimensional reaction-diffusion models with nearest neighbor interactions which can be exactly solved by EIM have been found and studied. Conditions have been obtained for the systems with finite reaction rates to be solvable via EIM, and then the equations of EIM have been solved. In [25], general conditions were obtained for a single-species reaction-diffusion system with nearest neighbor interactions, to be solvable through EIM. Here solvability means that evolution equation for E_n (the probability that n consecutive sites be empty) is closed. It turned out there, that certain relations between the reaction rates are needed, so that the system is solvable via EIM. The evolution equation of E_n is a recursive equation in terms of n , and is linear. It was shown that if certain reactions are absent, namely reactions that produce particles in two adjacent empty sites, the coefficients of the empty intervals in the evolution equation of the empty intervals are n -independent, so that the evolution equation can be easily solved. The criteria for solvability, and the solution of the empty-interval equation were generalized to cases of multi-species systems and multi-site interactions in [26–28].

In this article the most general single-species reaction-diffusion model with nearest-neighbor interactions on a Cayley tree is investigated, which can be solved exactly through the empty interval method. The scheme of the paper is as follows. In section 2, the most general reaction-diffusion model with nearest-

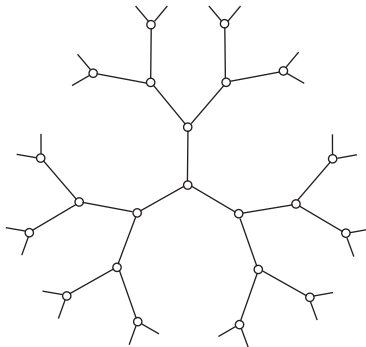


Figure 1: The Cayley tree with $\xi = 3$

neighbor interactions on a Cayley tree is studied, which can be solved exactly through EIM. The evolution equation of E_n is also obtained. In section 3 the stationary solution of such models, as well as their dynamics are discussed. Finally, section 4 is devoted to concluding remarks.

2 Models solvable through the empty interval method on a Cayley tree

The Cayley tree is a tree (a lattice without loops) where each site is connected to ξ sites (fig. 1). Two sites are called neighbors iff they are connected through a link. Consider a system of particles on a Cayley tree. Each site is either empty or occupied by one particle. The interaction (of particles and vacancies) is nearest neighbor. The probability that a connected collection of n sites be empty is denoted by E_n . It is assumed that this quantity does not depend on the choice of the collection. An example is a tree where the probability that a site is occupied is ρ and is independent of the states of other sites. Then

$$E_n = (1 - \rho)^n. \quad (1)$$

The following graphical representations help express various relations in a more compact form. An empty (occupied) site is denoted by \circ (\bullet). A connected collection of n empty sites is denoted by \bigcirc_n .

There is no loop in a Cayley tree, so each site can only be connected to a single existing cluster site, by a single link. For $\xi \geq 3$ (the case we are interested in here) the closedness of the evolution equation for E_n requires that the rate of creating an empty site be zero. The reason is that if it is not the case, then an empty n -cluster can be created from two disjoint empty clusters joined by a

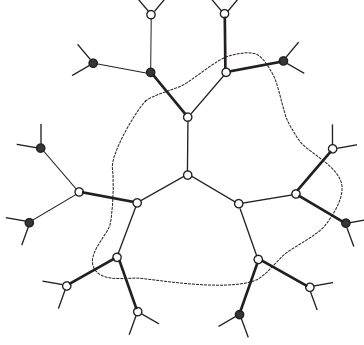


Figure 2: An empty cluster with the links at the boundary, on a Cayley tree with $\xi = 3$

single occupied site [29]. This shows that if the evolution of the empty clusters is to be closed, then the only possible reactions are the following, with the rates indicated.



(There is no distinction between left and right, of course.) This means that the reactants are immobile, and the coagulation and diffusion rates are zero.

Using these, one arrives at the following time evolution for E_n :

$$\begin{aligned}
 \frac{dE_n}{dt} &= -R_n r_1 P(\bullet\text{---}\bigcirc_n) - R_n (r_2 + r_3) P(\circ\text{---}\bigcirc_n) \\
 &\quad - (n-1)(2r_2 + r_3) P(\bigcirc_n),
 \end{aligned} \tag{3}$$

where R_n is the number of sites adjacent to a collection of n connected sites. A simple induction shows that

$$R_n = n(\xi - 2) + 2. \tag{4}$$

One has

$$P(\bullet\text{---}\bigcirc_n) + P(\circ\text{---}\bigcirc_n) = P(\bigcirc_n), \tag{5}$$

from which

$$P(\bullet\text{---}\bigcirc_n) = E_n - E_{n+1}. \tag{6}$$

Using this, one arrives at

$$\frac{dE_n}{dt} = R_n [-r_1 (E_n - E_{n+1}) - (r_2 + r_3) E_{n+1}] - (n-1) (2r_2 + r_3) E_n. \quad (7)$$

Throughout the paper, it is assumed that r_1 , r_2 , and r_3 are all nonzero.

3 The solution

The stationary solution of the system (E^s , for which the time derivative vanishes), satisfies

$$R_n [-r_1 (E_n^s - E_{n+1}^s) - (r_2 + r_3) E_{n+1}^s] - (n-1) (2r_2 + r_3) E_n^s = 0. \quad (8)$$

As E_n 's are nonnegative and nonincreasing in n , it is easy to see that the only solution to (8) is

$$E_n^s = 0. \quad (9)$$

This means that in the stationary configuration, all of the sites are occupied, which is not a surprise since in all reactions particles are created.

Regarding dynamics, one question is to obtain the spectrum of the evolution Hamiltonian. This is equivalent to finding solutions with exponential time dependence:

$$E_n^\mathcal{E}(t) = E_n^\mathcal{E} \exp(\mathcal{E} t). \quad (10)$$

Putting this in (7), one arrives at

$$- [R_n r_1 + (n-1) (2r_2 + r_3) + \mathcal{E}] E_n^\mathcal{E} + R_n (r_1 - r_2 - r_3) E_{n+1}^\mathcal{E} = 0. \quad (11)$$

From this,

$$E_{n+1}^\mathcal{E} = \zeta_n E_n^\mathcal{E}, \quad (12)$$

where

$$\zeta_n := \frac{R_n r_1 + (n-1) (2r_2 + r_3) + \mathcal{E}}{R_n (r_1 - r_2 - r_3)}. \quad (13)$$

It is seen that

$$\lim_{n \rightarrow \infty} \zeta_n = \frac{(\mathcal{E} - 2) r_1 + 2r_2 + r_3}{(\mathcal{E} - 2) (r_1 - r_2 - r_3)}. \quad (14)$$

The right-hand side is either negative or greater than one. So if all $E_n^\mathcal{E}$'s are nonzero, then $E_n^\mathcal{E}$'s either are not all nonnegative or blow up for large n 's. Such $E_n^\mathcal{E}$'s are not acceptable as probabilities. To see the reason, consider \mathcal{E}_1 (the largest \mathcal{E}). for large times, only E_n 's corresponding to this eigenvalue survive. But these should be nonincreasing with respect to n , and nonnegative, which is not the case. So $E_n^{\mathcal{E}_1}$'s must be identically zero for n larger than a certain integer (say n_1). A similar reasoning can then be made for \mathcal{E}_2 (the next largest value of \mathcal{E}), and the values of $E_n^{\mathcal{E}_2}$ for $n > n_1$, to show that there should be another integer n_2 so that $E_n^{\mathcal{E}_2}$ vanishes for $n > n_2$. This argument can be continued to show that for all \mathcal{E} 's, there must be an integer so that $E_n^\mathcal{E}$'s are identically

zero for n larger than that integer. This shows that ζ_n must be zero for some positive n , which gives the allowed values of \mathcal{E} :

$$\mathcal{E}_k = -\xi r_1 - (k-1)\beta, \quad k \geq 1, \quad (15)$$

where

$$\beta := (\xi - 2)r_1 + 2r_2 + r_3. \quad (16)$$

This spectrum is discrete, and there is a gap between the largest eigenvalue and zero, which means that the system evolves towards its stationary configuration with a relaxation time. This relaxation time is

$$\tau = \frac{1}{\xi r_1}. \quad (17)$$

One can also find $E_n^{\mathcal{E}}$'s. Denoting $E_n^{\mathcal{E}_k}$ by E_n^k , and using (12) and (15), one arrives at

$$E_n^k = \frac{\Gamma\left(k + \frac{2}{\xi - 2}\right) \alpha^{k-n}}{\Gamma\left(n + \frac{2}{\xi - 2}\right) (k-n)!}, \quad (18)$$

where

$$\alpha := \frac{(\xi - 2)(r_2 + r_3 - r_1)}{(\xi - 2)r_1 + 2r_2 + r_3}. \quad (19)$$

The general solution to (7) is then

$$E_n(t) = \sum_{k=1}^{\infty} c_k E_n^k \exp(\mathcal{E}_k t), \quad (20)$$

where c_k 's are to be determined from the initial condition.

A special solution to (7) is of the form

$$E_n(t) = E_1(t) [b(t)]^{n-1}. \quad (21)$$

Putting this in (7), one arrives at

$$\begin{aligned} \frac{db}{dt} &= -\beta b - \beta \alpha b^2, \\ \frac{dE_1}{dt} &= -\left(\xi r_1 + \frac{\xi}{\xi - 2} \alpha \beta b\right) E_1. \end{aligned} \quad (22)$$

These are readily solved and one obtains

$$\begin{aligned} b(t) &= \frac{b(0) \exp(-\beta t)}{1 + \alpha b(0) [1 - \exp(-\beta t)]}, \\ E_1(t) &= E_1(0) \exp(-\xi r_1 t) \left\{ \frac{1}{1 + \alpha b(0) [1 - \exp(-\beta t)]} \right\}^{\frac{\xi}{\xi - 2}}. \end{aligned} \quad (23)$$

Using these, one obtains

$$E_n(t) = E_n(0) \exp[-\xi r_1 t - (n-1) \beta t] \left\{ \frac{1}{1 + \alpha b(0) [1 - \exp(-\beta t)]} \right\}^{\frac{\xi}{\xi-2} + n-1}. \quad (24)$$

It is seen that for large times, all E_n 's tend to zero. In fact they decay like

$$E_n(t) \sim \exp[-\xi r_1 t - (n-1) \beta t]. \quad (25)$$

One notes that in fact $E_n(t)$ decays like $\exp(-\mathcal{E}_n t)$, and this is expected, as E_n^k is zero for $k < n$.

A special case where the ansatz (21) works is the case of initially uncorrelated-sites, so that each site is occupied with probability ρ regardless of other sites. One has then

$$E_n(0) = (1 - \rho)^n, \quad (26)$$

so that

$$\begin{aligned} E_1(0) &= 1 - \rho, \\ b(0) &= 1 - \rho. \end{aligned} \quad (27)$$

The special case $\xi = 2$ can be treated directly or as a limiting case of the general problem. The results corresponding to (15) and (18) would be

$$\mathcal{E}_k = -2 r_1 - (k-1) (2 r_2 + r_3), \quad \xi = 2, \quad (28)$$

and

$$E_n^k = \frac{1}{(k-n)!} \left[\frac{2(r_2 + r_3 - r_1)}{2 r_2 + r_3} \right]^{k-n}, \quad \xi = 2. \quad (29)$$

Finally, the solutions corresponding to the ansatz (21) would be

$$b(t) = b(0) \exp[-(2 r_2 + r_3) t], \quad \xi = 2, \quad (30)$$

and

$$\begin{aligned} E_1(t) &= E_1(0) \exp \left\{ \frac{2(r_1 - r_2 - r_3)}{2 r_2 + r_3} b(0) [1 - \exp[-(2 r_2 + r_3) t]] \right\} \\ &\times \exp(-2 r_1 t), \quad \xi = 2, \end{aligned} \quad (31)$$

so that

$$\begin{aligned} E_n(t) &= E_n(0) \exp \left\{ \frac{2(r_1 - r_2 - r_3)}{2 r_2 + r_3} b(0) [1 - \exp[-(2 r_2 + r_3) t]] \right\} \\ &\times \exp\{-[2 r_1 + (n-1) (2 r_2 + r_3)] t\}, \quad \xi = 2, \end{aligned} \quad (32)$$

4 Concluding remarks

The most general single-species exclusion model on a Cayley tree was considered, for which the evolution of the empty-intervals is closed. It was shown that in the stationary configuration of such models all sites are occupied. The dynamics of such systems were also studied and it was shown that the spectrum of the evolution Hamiltonian is discrete. The time evolution of the initially uncorrelated system was also obtained. Among the questions remaining, one can mention the problem of Cayley trees with boundaries, with injection and extraction at the boundaries.

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